

5«beta»-Androstan-3«alpha»-ol-17-one, TBDMS

Inchi:	InChI=1S/C31H58O2Si2/c1-28(2,3)34(9,10)32-23-17-19-30(7)22(21-23)13-14-24-25-15-
InchiKey:	CLHFTFZHTPFECO-AYEDRMSPSA-N
Formula:	C31H58O2Si2
SMILES:	CC12CCC3C(CCC4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	518.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.66		Crippen Method
logp	9.935		Crippen Method
rinpol	2698.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R526182&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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